

=> fil reg

FILE 'REGISTRY' ENTERED AT 15:30:29 ON 13 OCT 2004

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STRUCTURE FILE UPDATES: 12 OCT 2004 HIGHEST RN 761381-83-3

DICTIONARY FILE UPDATES: 12 OCT 2004 HIGHEST RN 761381-83-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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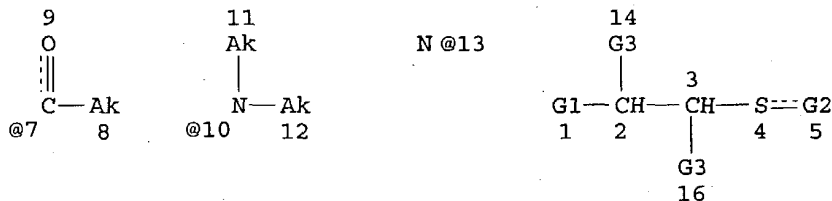
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 121

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L13 STR



VAR G1=10/13

VAR G2=CHO/7

VAR G3=AK/CY

NODE ATTRIBUTES:

NSPEC IS R AT 13

CONNECT IS M1 RC AT 13

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

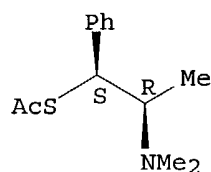
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1965:8904 CAPLUS
 DOCUMENT NUMBER: 62:8904
 ORIGINAL REFERENCE NO.: 62:1588a-c
 TITLE: Phenylmercaptoalkylamines. III. Hofmann degradation of
 1-phenyl-2-dimethylaminopropanethiol quaternary salts
 AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
 CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
 SOURCE: Yakugaku Zasshi (1964), 84(9), 811-17
 CODEN: YKKZAJ; ISSN: 0031-6903
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese
 AB Na2S2O3 and L-(+)-threo-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl,
 followed by hydrolysis, gave (+)-1-phenyl-2-dimethylaminopropanethiol (I),
 which was then converted into the methiodide and treated with NaOH to form
 (+)-1,2-epithiopropylbenzene (II), b10 100°, which was polymerized
 to give a polymer, m. 255-6°. Treatment of D-(+)-erythro-1,2-
 epoxypropylbenzene with KSCN gave L-(-)-erythro-1,2-epithiopropylbenzene,
 b7 92-3°, [α]20D-21.4° (c 2.21, MeOH), which was found
 to be the antipode of II. II belongs to the D-(+)-erythro series and I,
 to the L-(+)-threo series. The (-)-amino thiol, similarly derived from
 L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, was found
 to belong to the L-(-)-erythro series and that D-(+)-threo-1,2-
 epithiopropylbenzene (III) is derived from it. The steric configuration
 of II and III was also determined from their N.M.R. spectra. Hofmann
 degradation of the quaternary salt of 1-phenyl-2-dimethylaminoethanethiol
 also gave the same result. II and III underwent desulfurization by
 heating to give trans-β-methylstyrene.
 IT 1210-30-6, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-
 , acetate (ester), L-(-)-erythro-
 (preparation of)
 RN 1210-30-6 CAPLUS
 CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester,
 erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:497835 CAPLUS

DOCUMENT NUMBER: 131:350834

TITLE: Utilization of industrial waste materials. Part 14. Synthesis of β -amino alcohols and thiols with a 2-azabicyclo[3.3.0]octane backbone and their application in enantioselective catalysis

AUTHOR(S): Kossenjans, Michael; Soeberdt, Michael; Wallbaum, Sabine; Harms, Klaus; Martens, Jurgen; Aurich, Hans Gunter

CORPORATE SOURCE: Fachbereich Chemie, Universitat Oldenburg, Oldenburg, D-26129, Germany

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (16), 2353-2365

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:350834

AB New, chiral β -tert-amino tert-alcs. were synthesized from an enantiomerically pure sec-amine via glycine, alanine and phenylglycine derivs. Grignard addns. to these esters provided rigid amino alcs. in fair yields. The absolute configurations of the stereogenic centers, which arose during the alkylation step, were assigned by an independent route leading to some of the optical antipodes. The target compds. were derivs. of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol. Condensation of enantiomerically pure β -amino alcs. with a γ -keto ester afforded N,O-acetals which were subsequently reduced to the β -tert-amino alcs. X-Ray anal. of one compound was performed to verify the stereochem. observed by chemical correlation. The nucleophilic ring opening of enantiomerically pure styrene oxide by an amine resulted in the formation of regioisomeric amino alcs. Amino thiol derivs. were also prepared. Reduction of these compds. to thiols and subsequent oxidation afforded amino disulfides. Finally, the bicyclic β -amino alcs. and thiols were used as chiral ligands in the enantioselective addition of diethylzinc to benzaldehyde and ee values up to 96% were found.

IT 250371-17-6P

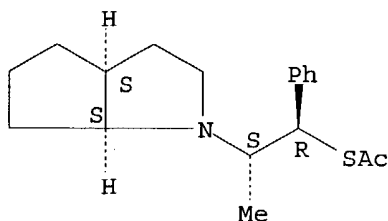
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

RN 250371-17-6 CAPLUS

CN Ethanethioic acid, S-[(1R,2S)-2-[(3aS,6aS)-hexahydrocyclopenta[b]pyrrol-1(2H)-yl]-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:569540 CAPLUS
DOCUMENT NUMBER: 129:289723
TITLE: Zirconocene-Zinc Transmetalation and in Situ Catalytic
Asymmetric Addition to Aldehydes
AUTHOR(S): Wipf, Peter; Ribe, Seth
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh,
Pittsburgh, PA, 15260, USA
SOURCE: Journal of Organic Chemistry (1998), 63(19), 6454-6455
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The in situ hydrozirconation of alkynes, trans-metalation to dimethylzinc and chiral amino thiol-catalyzed addition to aldehydes provided an efficient protocol for the asym. preparation of (E)-allylic alcs. For example, the hydrozirconation of 1-hexyne, followed by transmetalation via addition of dimethylzinc and sequential addition of the resulting (alkenyl)methylzinc intermediate to benzaldehyde gave [S-(E)]-1-phenyl-2-hepten-1-ol [i.e., [S-(E)]- α -(1-hexenyl)benzenemethanol] in 90% and in 83% enantiomeric excess. The last step in the sequence was catalyzed in the presence of (R)-2-[1-(dimethylamino)propyl]benzenethiol as ligand.

IT 185606-94-4

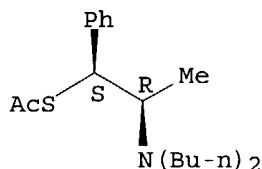
RL: CAT (Catalyst use); USES (Uses)

(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to aldehydes)

RN 185606-94-4 CAPLUS

CN Ethanethioic acid, S-[(1S,2R)-2-(dibutylamino)-1-phenylpropyl] ester (9CI)
(CA INDEX NAME)

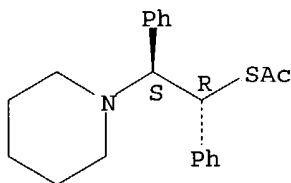
Absolute stereochemistry.



REFERENCE COUNT:

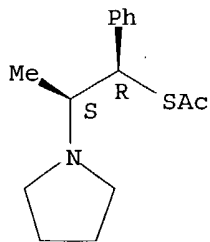
ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1997:39785 CAPLUS
 DOCUMENT NUMBER: 126:131036
 TITLE: Chiral β -amino thiol catalysts for the
 enantioselective addition of diethylzinc to aldehydes
 AUTHOR(S): Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong
 Soo; Kim, Joo In
 CORPORATE SOURCE: Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea
 SOURCE: Bulletin of the Korean Chemical Society (1996),
 17(12), 1135-1142
 CODEN: BKCSDE; ISSN: 0253-2964
 PUBLISHER: Korean Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Reaction of diethylzinc with α -branched aldehydes in the presence of
 a catalytic amount (5 mol %) of various β -amino thiols in toluene or
 ether provided the corresponding secondary alcs. in outstanding ee.
 Detailed preparative procedure for the β -amino thiols are presented.
 IT 160011-79-0P 166031-45-4P 166031-48-7P
 186314-11-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (enantioselective addition of diethylzinc to aldehydes using chiral
 β -amino thiol catalysts)
 RN 160011-79-0 CAPLUS
 CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-piperidinyl)ethyl] ester
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



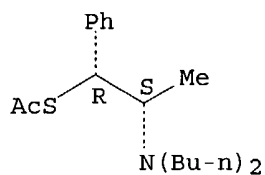
RN 166031-45-4 CAPLUS
 CN Ethanethioic acid, S-[1-phenyl-2-(1-pyrrolidinyl)propyl] ester,
 [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



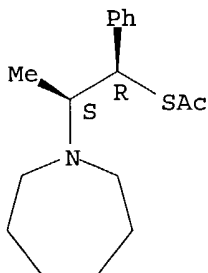
RN 166031-48-7 CAPLUS
 CN Ethanethioic acid, S-[2-(dibutylamino)-1-phenylpropyl] ester, [R-(R*,S*)]-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



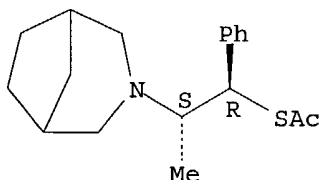
RN 186314-11-4 CAPLUS
 CN Ethanethioic acid, S-[2-(hexahydro-1H-azepin-1-yl)-1-phenylpropyl] ester,
 [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 186314-19-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (enantioselective addition of diethylzinc to aldehydes using chiral
 β-amino thiol catalysts)
 RN 186314-19-2 CAPLUS
 CN Ethanethioic acid, S-[2-(3-azabicyclo[3.2.1]oct-3-yl)-1-phenylpropyl]
 ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:729946 CAPLUS

DOCUMENT NUMBER: 126:103872

TITLE: New chiral catalysts for the highly enantioselective addition of diethylzinc to aldehydes

AUTHOR(S): Jin, Myung-Jong; Ahn, Sum-Jin; Lee, Kyoung-Soo

CORPORATE SOURCE: Dep. Chemical Engineering, Inha Univ., Incheon, 402-751, S. Korea

SOURCE: Tetrahedron Letters (1996), 37(48), 8767-8770

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Optically active amino thioacetate derivs. of (+)-norephedrine were found to act as effective catalysts for enantioselective addition of diethylzinc to aldehydes. This reaction provided optically active secondary alcs. with e.e. of up to >99%.

IT 185606-97-7

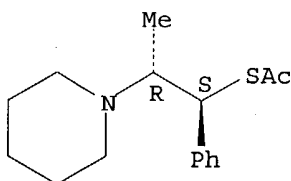
RL: CAT (Catalyst use); USES (Uses)

(chiral catalysts for enantioselective addition of diethylzinc to aldehydes)

RN 185606-97-7 CAPLUS

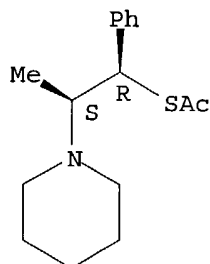
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



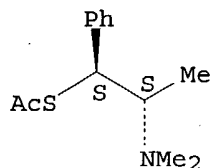
ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1995:86424 CAPLUS
 DOCUMENT NUMBER: 123:142957
 TITLE: Enantioselective addition of diethylzinc to α -branched aldehydes
 AUTHOR(S): Kang, Jahyo; Lee, Jun Won; Kim, Joo In
 CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
 SOURCE: Journal of the Chemical Society, Chemical Communications (1994), (17), 2009-10
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Reaction of diethylzinc with α -branched aldehydes in the presence of a catalytic amount of (1R,2S)-(-)-1-phenyl-2-piperidinopropane-1-thiol provided the corresponding secondary alcs. in almost 100% enantiomeric excess.
 IT **166031-44-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthetic intermediate; in conversion to ligand catalyst for enantioselective addition of diethylzinc to α -branched aldehydes)
 RN 166031-44-3 CAPLUS
 CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:680925 CAPLUS
 DOCUMENT NUMBER: 121:280925
 TITLE: Nucleophilic substitutions using O-alkyl-N,N'-
 dialkylisoureas. Applications to ephedrine
 AUTHOR(S): Poelert, Martin A.; Hulshof, L. A.; Kellogg, Richard
 M.
 CORPORATE SOURCE: Dep. Organic Chemi., Univ. Groningen, Groningen, 9747
 AG, Neth.
 SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1994),
 113(7-8), 365-8
 CODEN: RTCPA3; ISSN: 0165-0513
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 121:280925
 AB Dialkylcarbodiimides in the presence of a CuI catalyst react cleanly with
 the hydroxyl group of N-methylated (1R,2S)-ephedrine and
 (1S,2S)-pseudoephedrine. These adducts react with nucleophiles like alkyl
 and aryl thiols as well as thioic acids and phthalimide to form the
 substitution products with overall retention of configuration. It is
 postulated that intramol. participation of the amino group via an SN2
 reaction leads to aziridinium salts, which are subsequently opened by the
 nucleophiles via a second SN2 reaction. This synthetic approach is also
 useful for the inversion of simple secondary alcs.; on treatment with
 dicyclohexylcarbodiimide followed by benzoethioic acid and treatment with
 LiAlH4, menthol was converted in good yield to neomenthane thiol.
 IT 2226-22-4P 2226-23-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (nucleophilic substitutions using alkyl dialkylisoureas, applications to
 ephedrine)
 RN 2226-22-4 CAPLUS
 CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester,
 [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 2226-23-5 CAPLUS
 CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester,
 [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

